

# **Local Structure of Silica Zeolite ITQ-4 Loaded With Cs**

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Beamline(s): X7A

**Introduction:** Electrides are strongly reducing materials in which alkali metals (Li through Cs) ionize to form bound alkali cations and 'excess' electrons. The electrons reside in large cavities in the host lattice to form an 'electron lattice gas'. A long-standing goal of the electride research has been to synthesize inorganic electrides that are thermally stable at and above room temperature. We report a study on the local structure of silica zeolite ITQ-4,  $\text{Si}_{32}\text{O}_{64}$ , loaded with cesium that may provide the first true inorganic electride.

**Methods and Materials:** The zeolite used in this work has a rather open structure with sinusoidal channels of diameter  $\sim 7 \text{ \AA}$  running in one direction. Since ITQ-4 contains no cations initially, loading with Cs would yield one electron per cation. The amount of Cs that can be introduced *in vacuo* from the vapor phase varies from zero to 40 %. Of major interest is the nature of Cs species formed in the channels. We addressed the issue by studying three samples, pristine  $\text{Si}_{32}\text{O}_{64}$ ,  $\text{Cs}_{3.6}\text{Si}_{32}\text{O}_{64}$  and  $\text{Cs}_{4.6}\text{Si}_{32}\text{O}_{64}$ . The experiments were carried out at the beamline X7A, NSLS, Brookhaven.

**Results:** Experimental powder diffraction spectra are shown in Fig. 1. As can be seen the incorporation of Cs introduces significant structural disorder. This makes it necessary to reduce the data to the corresponding atomic pair distribution functions (PDF). These are shown in Fig. 2. Structure modeling based on the experimental PDFs is under way. The outcomes will be reported elsewhere.

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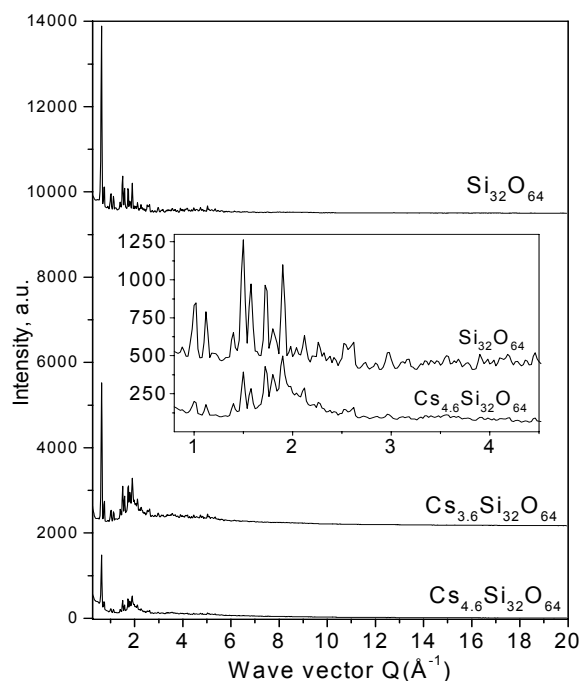


Figure 1. Powder diffraction patterns of pristine and Cs loaded ITQ-4. Data are shown in an expanded scale in the inset.

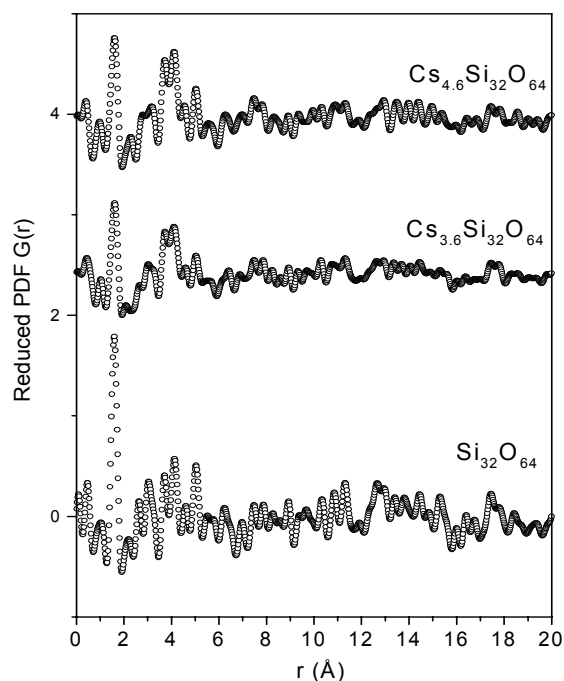


Figure 2. Experimental PDFs for pristine and Cs loaded ITQ-4.